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# SIMULATION OF CARBON NANOTUBES FOR HYDROGEN STORAGE USING NEURAL NETWORK: A PRELIMINARY STUDY

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## ABSTRACT

The discovery of carbon nanotubes (CNT) by Sumio Iijima in 1991 has attracted many researchers worldwide to study and explore the newly found materials. The unique characteristics that CNT possess include excellent properties for energy production and hydrogen storage. Currently, there are 4 technologies available for hydrogen storage: compressed gas, liquefaction, metal hydrides and physisorption. It has been claimed that physisorption is the most promising hydrogen storage method for meeting the goals of the US Department of Energy (DOE) Hydrogen Plan for fuel cell powered vehicles. CNT are considered for hydrogen storage due to their low density, high strength, and hydrogen adsorption characteristics. A number of theoretical and experimental investigations have been made in this area mainly to study whether CNT can reach the benchmark of gravimetric density of 6.5 wt% and volumetric density of 62 kg $H_2/m^3$ set by the DOE Hydrogen Plan. Based on previous researches, a numerical simulation of CNT for hydrogen storage using Artificial Neural Network (ANN) will be developed.

Keywords: carbon nanotubes; neural network; simulation

## ABSTRAK

Penemuan nanotiub karbon oleh Sumio Iijima pada tahun 1991 telah menarik minat para penyelidik di seluruh dunia untuk menjalankan kajian mengenai bahan yang baru ditemui itu. Sifat-sifat unik yang dimiliki oleh nanotiub karbon telah membuatkan ia dipertimbangkan sebagai salah satu bahan untuk menghasilkan tenaga dan juga untuk menyimpan hidrogen. Pada ketika ini terdapat 4 teknologi yang sedang dibangunkan untuk menyimpan hidrogen iaitu kaedah pemampatan gas, kaedah pencairan, logam terhidrat dan penjerapan gas. Para penyelidik meramalkan bahawa kaedah penjerapan gas merupakan satu cara yang menjanjikan kadar penyimpanan hidrogen yang terbaik setakat ini di mana ia dapat menghampiri sasaran yang telah ditetapkan oleh Rancangan Hidrogen Jabatan Tenaga US (DOE) bagi kenderaan yang menggunakan sel bahan api sebagai penjana kuasanya. Nanotiub karbon dipertimbangkan sebagai penyimpan hidrogen disebabkan oleh sifat-sifat yang dimiliki olehnya seperti mempunyai kepadatan yang rendah tetapi pada waktu yang sama mempunyai daya kekuatan yang tinggi di samping memiliki kebolehan untuk menjerap hidrogen. Pelbagai teori dan eksperimen telah dibuat oleh para penyelidik bagi mengkaji sekiranya nanotiub karbon dapat menghampiri sasaran "gravimetric density"sebanyak 6.5% dan "volumetric density" sebanyak $62kgH_2/m^3$ yang ditetapkan oleh DOE. Berdasarkan data-data dari kumpulan penyelidik terdahulu, satu simulasi yang menggunakan sistem Neural Network akan dibangunkan untuk mengkaji nanotiub karbon sebagai penyimpan hidrogen.


Katakunci: nanotiub karbon; neural network; simulasi

## INTRODUCTION

The new form of carbon called carbon nanotubes (CNT) was first discovered by Sumio Iijima in 1991. Ever since that day, many research groups have been devoted to studying this new material. CNT is a cylindrical molecule approximately 1nm in diameter and 1-100 micron in lengths and constituted of carbon only. It can also be thought of as a layer of graphite rolled-up into a cylinder. There are 2 types of CNT, single-walled carbon nanotubes (SWNT) and multi-walled carbon nanotubes (MWNT). SWNT is tubes formed by only one single graphite layer while MWNT is tubes containing of multiple concentric graphite layers. The diameter of SWNT rises from 0.671 to 3nm. MWNT show typical diameter of 30-50nm. The unique electronic and mechanical properties of CNT make them a very versatile material. Among its applications are as field emission sources, Atomic Force Microscope (AFM) tips, rectifying diodes and transistors. Bulk quantities of nanotubes are also useful as high-capacity hydrogen storage media for fuel cell vehicle.

Since the discovery of hydrogen storage capacity CNT, many researches have been conducted in this area as hydrogen is expected to replace the existing conventional fuel in the future. Hydrogen is the most promising candidate to replace the current fossil fuel since it is not only environmentally compatible (pollution-free), but it also can be produced from renewable energy sources, thus eliminating the net production of greenhouse gases. Despite tremendous efforts to use hydrogen as a source of energy, a safe and efficient on board storage technology has never been easily accessible. Due to its explosiveness, an efficient storage method is needed for hydrogen to become a replacement for fossil fuels. The discovery of the hydrogen storage capacity of CNT makes such a method very promising. Nevertheless, certain requirements have to be fulfilled before a feasible on board hydrogen storage system can be developed. The US Department of Energy (DOE) Hydrogen Plan has set a standard for fuel cell powered vehicle by requiring a gravimetric density of 6.5wt% and a volumetric density of 62kg $H_2/m^3$.

In general, there are 4 main technologies being explored for hydrogen storage: Compressed gas, liquefaction, metal hydrides and physisorption (gas-on-solid adsorption). Although nowadays all of these options are investigated extensively and progress is gained, none of these technologies is fully developed. There are still some significant disadvantages which exists. For example, the critical issue connected with compressed gas storage may be tank volume and safety, while liquefying hydrogen wastes at least 1/3 of stored energy and suffers from potential losses due to evaporation and the hydride-based approach suffers from weight and cost concerns. The storage based on physisorption potentially may have a higher energy density. It has been claimed that physisorption is the most promising hydrogen storage method for meeting the goals of the DOE Hydrogen Plan for fuel cell powered vehicle. Physisorption is an inherently safe and potentially high energy density $H_2$ storage method that could be extremely energy efficient.

Due to the scientific, technological and economical potential of CNT on hydrogen storage, a number of theoretical and experimental investigations have been made. Based on the data from the experiments by other researchers, a numerical simulation of CNT for hydrogen storage is expected to be developed using Artificial Neural Network (ANN). Neural network is a type of Artificial Intelligence that is inspired by the way the brain process information. It is composed of a large number of highly interconnected processing elements (neurons), working in parallel to solve specific problem.

ANN research has experienced three periods of extensive activity. The first peak was in the 1940s due to McCulloch and Pitts' pioneering work. The second occurred in 1960s with Rosenblatt's perceptron convergence theorem and Minsky and Papert's work showing the limitations of a simple perceptron. Even though Misky and Papert's results dampened the enthusiasm of most researchers, a major development emerged in 1980s when Hopfield came with his energy approach in 1982.

ANN can be viewed as weighted directed graphs in which artificial neurons are nodes and directed edges (with weights) are connection between neuron outputs and neuron inputs. Figure 1 below shows typical network for a multilayer perceptron with 3-layer. The input layer consists of neurons that receive input from the user. The output layer consists of neurons that communicate the output of the system to the user. There are usually a number of hidden layers between these 2 layers. Figure 1 shows a simple structure with only one hidden layer. When the input layer receives the input, its neurons produce output, which becomes input to the other layer of the system. The process continues until a certain condition is satisfied or until the desired output is reached.

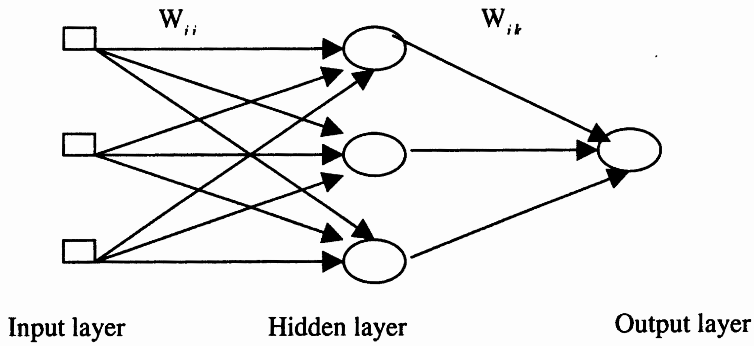


FIGURE 1 Neural Network Architecture

Basically, there are two learning paradigms of neural network: supervised learning system and unsupervised learning system. Supervised learning system models how ANN system can learn about their environments when the correct result (desired output) are known and are given to the ANN during training. It is usually used as calculation tools. Unsupervised learning system models how ANN system can learn about their environment without explicit feedback. The ANN is not provided with the correct results during training. Unsupervised ANN usually performs some bound of data compression, such as dimensionally reduction or clustering. Its application including recognition of images and speech signals.

## METHODS

A learning process in the ANN context can be viewed as the problem of updating network architecture and connection weights so that a network can efficiently perform a specific task. The network usually must learn the connection weights from available training patterns. Performance is improved over time by updating the weights in the network iteratively. ANN appears to learn the underlying rules from the given collection of representative examples.

Various aspects have to be considered before a satisfactory model of neural network can be developed. The development of Neural Network model is including:

a) Arranging neurons in various layers
b) Deciding the type of connections among neurons for different layers, as well as among the neurons within a layer
c) Deciding the way a neuron receives input and produces output
d) Determining the strength of a connection within the network by allowing the network learn the appropriate values of connections weight by using a training data set

A trial and error period in the design decisions would be carried out before a satisfactory design is found.

## RESULT AND DISCUSSION

From the numerical and experimental investigation's result, there is no common conclusion for maximum adsorption capacity of hydrogen in carbon nanotubes. However, based on the literature review, a mathematical model that would predict the hydrogen storage capacity based on the geometry and physical characteristics of CNT would be developed. A numerical simulation of CNT for hydrogen storage using Artificial Neural Network (ANN) will also be developed. MATLAB will be used as a platform to create the network.

## CONCLUSION

Throughout the project, factors that affect the adsorption capacity of hydrogen in carbon nanotubes will be identified. The mathematical model of the adsorption of hydrogen onto CNT as well as a neural network system that can be used to simulate CNT as hydrogen storage will also be developed.

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